201-14938A

Fyrol 6
HPV TEST PLAN

Submitted to the U.S. Environmental Protection Agency

By

Akzo Nobel Functional Chemicals LLC

December 2003

TABLE OF CONTENTS

LIST OF TABLES

SUMMARY

Akzo Nobel Functional Chemicals LLC has sponsored phosphonic acid, [[bis (2-hydroxyethyl) amino] methyl]- diethyl ester (CAS# 2781-11-5), also known as Fyrol 6, in the U.S. EPA High Production Volume (HPV) program.

Robust summaries of studies on Fyrol 6 are included in this submission. The table below summarizes the endpoints of interest in the HPV program, the available data, and indicates proposed testing.

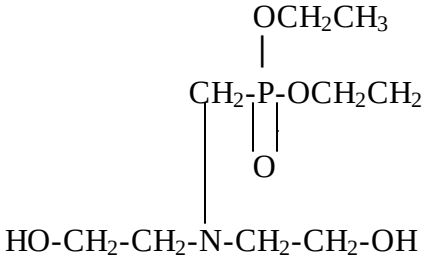
Endpoint	Data Available & Sufficient	Testing Proposed
Physical/Chemical Characteristics		
Melting Point	No	Yes
Boiling Point	Yes	No
Vapor Pressure	Yes	No
Water Solubility	Yes	No
Octanol:Water Partition Coefficient	Yes	No
Photodegradation	Yes	No
Hydrolysis	No	Yes
Biodegradation	Yes	No
Transport	Yes	No
Acute Fish Toxicity	Yes	No
Acute Daphnia Toxicity	No	Yes
Acute Alga Inhibition	No	Yes
Acute Toxicity	Yes	No
Genetic Toxicity	Yes	No
Repeated Dose	Yes	No
Reproductive Toxicity	No	Yes (OECD 421)
Developmental Toxicity	No	Yes (OECD 421)

1.0 INTRODUCTION

Akzo Nobel Functional Chemicals LLC has sponsored phosphonic acid, [[bis (2-hydroxyethyl) amino] methyl]- diethyl ester (CAS# 2781-11-5), also known as Fyrol 6, in the U.S. EPA High Production Volume (HPV) program. Fyrol 6 is a flame retardant that is reacted into rigid polyurethane foam.

This document includes an evaluation of the available toxicity data and test plan. It is proposed that a melting point study, hydrolysis study, acute aquatic invertebrate and algae studies as well as a reproductive/developmental toxicity screening study (OECD 421) be conducted.

Fyrol 6



2.0 USE AND EXPOSURE

Fyrol 6 is manufactured at one site in a closed system in which worker exposure is limited to sampling, analysis in the laboratory and drumming operations. Shipments are typically done in 55 gallon drums and occasionally in bulk tank trucks. Disposal of Fyrol 6 at the manufacturing site is done in a closed wastewater treatment system. Fyrol 6 is used primarily as a flame retardant for urethane and electronic laminate resin systems. Handling by the customer is done via a closed system metered into the resin system during manufacture. Fyrol 6 reacts with and becomes an integral part of the resin system during production. Any worker exposure at the customer's site is during sampling and opening of product containers before processing. Disposal is typically carried out by washing and wastewater treatment.

3.0 EVALUATION OF EXISTING DATA AND PROPOSED TESTING

The available data for Fyrol 6 have been evaluated below and summarized in Tables 1-3. Robust summaries of the studies are included in this submission. The Klimisch reliability code was used in the robust summaries. A literature search on Fyrol 6 of online data bases including TOXLINE, HSDB and RTECS was conducted. There were no relevant studies identified. Fyrol 6 is an amine phosphorous chemical for which there are no structural analogs.

Physical/Chemical Properties:

The melting point for Fyrol 6 is estimated by the EPIWIN model to be 83.21°C. Fyrol 6 is a liquid so the estimation is inaccurate. The boiling point using the EPIWIN model for Fyrol 6 is 379.37°C. The vapor pressure of Fyrol 6 is 0.43 mmHg at 20°C. The log octanol:water partition coefficient (log Kow) of Fyrol 6 is –0.72. The water solubility of Fyrol 6 is 900 g/L.

Recommendation: Testing for melting point is proposed.

Environmental Fate:

AOPWIN was used to estimate the chemical half-life based on an overall OH reaction rate constant. Photodegradation modeling results for Fyrol 6 indicate the half-life is estimated to be 0.898 hours.

Hydrolysis data are not available.

The EPIWIN Level III fugacity model was used to estimate the distribution of Fyrol 6. The modeling results indicate that Fyrol 6 primarily distributes to water and soil.

Fyrol 6 was biodegraded 19% at day 28 of a Modified Sturm Test. It is considered not readily biodegradable.

Recommendation: Testing for hydrolysis is proposed.

Aquatic Toxicity:

The 96 hour LC50 in fish for Fyrol 6 is greater than 10000 mg/L.

Recommendation: Acute testing in Daphnia magna and algae are proposed.

Acute Toxicity:

The acute oral and dermal LD50 values in rats and rabbits for Fyrol 6 are greater than 5000 and 2000 mg/kg, respectively. Fyrol 6 was not irritating to rabbit skin following a 4 hour exposure. It was mildly irritating to rabbits in an eye irritation study.

Recommendation: No additional testing is proposed.

Repeated Dose:
The NOAEL for Fyrol 6 in a 13 week oral gavage study in rats was 500 mg/kg/day. Minor histopathological changes in the liver were seen at 100 and 500 mg/kg/day. The authors of the report suggested that this effect was due to an adaptive response and not the test article.

Recommendation: No additional testing is proposed.

Reproductive/Developmental Toxicity:

There have been no reproductive or developmental toxicity studies conducted on Fyrol 6.

Recommendation: A reproductive/teratology screening study (OECD 421) is proposed for Fyrol 6.

Mutagenicity:
Fyrol 6 was not mutagenic in the Ames test and was negative in the BALB/3T3 cell transformation assay. Fyrol 6 was mutagenic in the mouse lymphoma forward mutation assay and was clastogenic in the mouse lymphoma chromosome aberration study.

Recommendation: No additional testing is proposed.

TABLE 1: PHYSICAL/CHEMICAL DATA

CAS #	Chemical (Mol. Weight)	MW	MP °C	BP °C	Vapor pressure (mmHg)	Water Sol. (g/L)	Log Kow	Phys. Appear.
2781-11-5	Fyrol 6 (255)	216	Test	379.37[a]	0.43	900	-0.72	Clear amber liquid

[a] Data from EPIWIN

TABLE 2: SUMMARY OF ENVIRONMENTAL FATE AND ECOTOXICITY DATA

CAS #	Chemical (Mol. Weight)	Environmental Fate				Ecotoxicity LC50/EC50 (mg/L)		
		Photodeg (hr.).	Stability in water (25°C)	Biodeg.	Trans./ Distr.	Fish	Invert.	Plants
2781-11-5	Fyrol 6 (255)	0.898[a]	Test	Not readily biodegradable	Primarily to soil/water[a]	> 10,000	Test	Test

[a] Data from EPIWIN

TABLE 3: SUMMARY OF MAMMALIAN TOXICITY DATA

CAS #	Chemical (Mol. Weight)					Genetic toxicty	
		Acute (g/kg)	Repeated dose	Reproductive	Develop.	Mutagen.	Chrom. Aberr.
2781-11-5	Fyrol 6 (255)	>5 (oral) >2 (dermal)	NOAEL – 500 mg/kg/day (13 week)	Test (OECD 421)	Test (OECD 421)	Ames- not mutagenic ; Transformation assay – negative ; Mouse lymph. - mutagenic	Mouse lymph. - clastogenic